

AMENDMENTS TO THE SPECIFICATION:

Please replace the Title at Page 1, lines 1-2 with the following amended title:

METHOD AND APPARATUS FOR DETERMINING MOLECULAR CRYSTAL STRUCTURES

Please replace the paragraph at page 4, lines 9-18 with the following amended paragraph:

Moreover, preferably, the fitness χ^2 of each of the trial structures is determined using the following function:

$$\chi^2 = \sum_h \sum_k \{(\mathbf{I}_h - \mathbf{c} | \mathbf{F}_h|^2) (\mathbf{V}^{-1})_{hk} (\mathbf{I}_k - \mathbf{c} | \mathbf{F}_k|^2)\}$$

where:

$\mathbf{I}_h, \mathbf{I}_k$ = extracted intensity

$\mathbf{V}_{h,k}$ = covariance matrix

\mathbf{c} = a scale factor

$\mathbf{F}_h, \mathbf{F}_k$ = calculated structure factor from trial structure

Please replace the paragraph at page 10, line 32, to page 11, line 14 with the following amended paragraph:

Using the internal co-ordinates a three dimensional structure of the trial molecule is constructed (35) for each parent in Cartesian space, and then in fractional space with respect to the crystal unit cell. Diffraction data is then determined (37) for each of the trial molecular structures and a fitness value, χ^2 , is calculated (39) for each trial structure with respect to the structure factor intensity listing and covariance matrix. The preferred fitness function employed is as follows:

$$\chi^2 = \sum_h \sum_k \{(\mathbf{I}_h - \mathbf{c} | \mathbf{F}_h|^2) (\mathbf{V}^{-1})_{hk} (\mathbf{I}_k - \mathbf{c} | \mathbf{F}_k|^2)\}$$

where:

$\mathbf{I}_h, \mathbf{I}_k$ = extracted intensity

$\mathbf{V}_{h,k}$ = covariance matrix

\mathbf{c} = a scale factor

$\mathbf{F}_h, \mathbf{F}_k$ = calculated structure factor from trial structure